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NONEQUILIBRIUM RADIATION AND CHEMISTRY MODELS *p 33*
FOR AEROCAPTURE VEHICLE FLOWFIELDS

Volume III

aerospace
engineering
department



Semiannual Progress Report
July 1990 -- December 1990

TEXAS A&M UNIVERSITY

TAMRF Report No. 6382-91-01-(III)

February 1991

(NASA-CR-188195) NONEQUILIBRIUM RADIATION
AND CHEMISTRY MODELS FOR AEROCAPTURE VEHICLE
FLOWFIELDS, VOLUME 3 Semiannual Progress
Report, Jul. - Dec. 1990 (Texas A&M Univ.)
33 p

N91-24102

Unclassified
0012586

NASA Grant No. NAG-1-1003

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TEXAS ENGINEERING EXPERIMENT STATION

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USER'S MANUAL FOR THE PRECURSOR SOLUTION SCHEME
(Programs: RADICAL, PREC, CHKCONV, etc.)

by

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for

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December 1990

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INTRODUCTION

This document describes the computer programs developed to calculate the shock wave precursor and the method of using them. This method calculates the precursor flow field in a nitrogen gas including the effects of emission and absorption of radiation on the energy and composition of the gas. The radiative transfer is calculated including the effects of absorption and emission through the line as well as the continuum processes in the shock layer and through the continuum processes only in the precursor. The effects of local thermodynamic nonequilibrium in the shock layer and precursor regions are also included in the radiative transfer calculations. Details of the formulation of this computational method are provided in the thesis by Stanley¹.

This computational scheme utilizes three computer programs to calculate the precursor flow field solution for a given shock layer flow field. The first of these programs, RADICAL, is used to calculate the radiative transfer through the flow field. This program is a modified version of a program written by Nicolet^{2,3}. The second program, PREC, calculates the precursor flow field utilizing the radiative transfer results from RADICAL. In order to calculate a precursor flow field solution it is necessary to iterate between the two programs, RADICAL and PREC, to fully couple the radiative transfer and the precursor flow field. This iterative scheme will be discussed in the next section.

Finally, CHKCONV calculates the maximum change between two precursor flow field solutions. This program is used to check for convergence of the precursor flow field and the radiative transfer in the iteration between RADICAL and PREC.

There are also a number of programs which can be used to manipulate the output files from this solution method. These programs will be discussed in the final section of this text.

SOLUTION SCHEME

As discussed above, it is necessary to iterate between the two programs, RADICAL and PREC, in order to calculate a coupled precursor solution. This iteration is necessary since the precursor flow field is dependent on the radiative transfer and is also necessary to correctly calculate the radiative transfer.

This iteration scheme begins by first assuming a set of flow field conditions in the precursor. RADICAL is then used to calculate the radiative transfer through the entire flow field utilizing these precursor conditions along with the known shock layer conditions. These radiative transfer results are then utilized by the program PREC in the calculation of a new precursor flow field. Finally, the program CHKCONV is used to compare the new precursor flow field to the previous flow field to check for convergence. This iterative scheme is illustrated graphically in Figure 1.

Appendix A is a command file which iterates through this solution scheme five times. It has been found through numerical studies that five iterations will typically meet a convergence criteria of 0.05 percent. This command file saves all five of the precursor flow field solutions in the files prec1.dat, prec2.dat, ..., prec5.dat.

Details on the input and output files for each individual program are provided in the following sections.

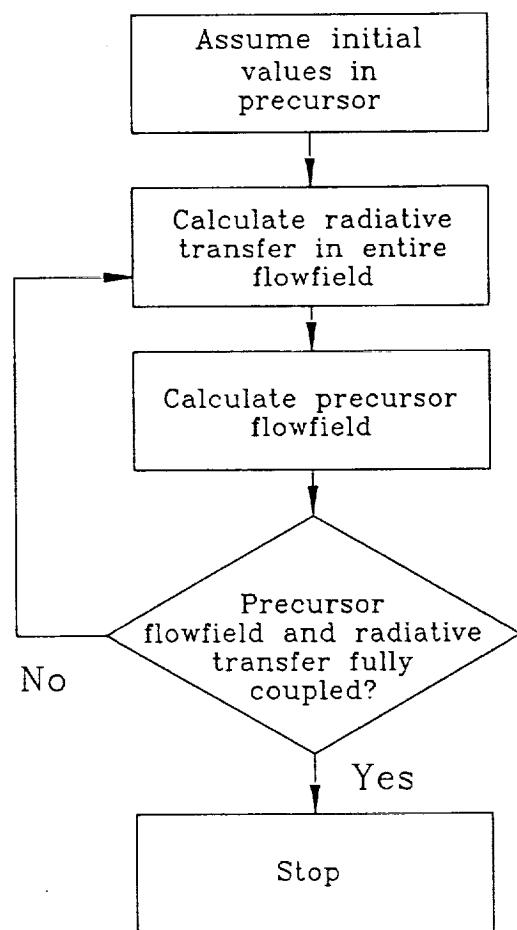


Figure 1: Precursor Iteration Scheme

RADICAL

As mentioned previously, RADICAL is a modified version of a radiative transfer program written by Nicolet². In order to use this program it was necessary to modify some subroutines in order to extract the information necessary to calculate the radiative effect on the precursor flow field. Also, several radiative processes which are important in the cool nitrogen precursor have been added to those originally included in RADICAL. These modifications involved changes in the six subroutines:

contn	lint
contn2	lint2
mu	mule

and the main routine,

radical

The subroutine, addlns, was also added during these modifications.

Changes have also been made to RADICAL to include collision limiting⁴ corrections for local thermodynamic nonequilibrium in the precursor region. These modifications include changes to the subroutines contn2 and mu as well as the addition of eleven subroutines:

ai3	gami
ai3a	limit
crosab	molin
exctml	parim
exctmm	taint
gamc	

It should also be noted that the dimension statements in RADICAL have been modified to allow 300 spatial points.

INPUT FILES

RADICAL reads from four input files:

fort.24	rad.dat
prec.dat	fort.3

The first two of these files, fort.24 and prec.dat, contain the shock layer and the precursor flow field conditions, respectively.

fort.24 - Shock layer flow field data, see Appendix B.

Line 1, [I5, 9E13.6]

Field 1, (Columns 1-5) JE

The number of spatial points used in the shock layer, maximum of JE + JPREC = 300.

Field 2, (Columns 6-18) S

S location around the body in the VSL solution. Not used in the precursor calculations.

Field 3, (Columns 19-31) YS(2)

Shock layer thickness nondimensionalized by the body nose radius,
 $YS(2) = Y_{shock}/R_{nose}$.

Field 4, (Columns 32-44) RNOSE

Body nose radius, R_{nose} (ft).

Field 5, (Columns 45-57) TREF

Reference temperature in the VSL nondimensionalization scheme
 $(^{\circ}R)$.

Field 6, (Columns 58-70) PREF

Reference pressure in the VSL nondimensionalization scheme (psi).

Field 7, (Columns 71-83) PS(2)

Nondimensional pressure immediately behind the shock,
 $PS(2) = P_{behind\ shock}/PREF$

Field 8, (Columns 84-96) RHOREF

Reference density in the VSL nondimensionalization scheme
 $(\text{slug}/\text{ft}^3)$.

Field 9, (Columns 97-109) RS(2)

Nondimensional density immediately behind the shock,
 $RS(2) = \rho_{behind\ shock}/RHOREF$.

Field 10, (Columns 110-122) TWALL

Wall temperature for use in the radiative flux calculations ($^{\circ}R$).

Line 2, [I5, 9E13.6]

Field 1, (Columns 1-5) NS

Number of species in gas.

Field 2, 3, ..., NS, (Columns 6-18, 19-31, etc) (EMI(j), j=1, NS)
 Molecular weight of the jth species, (g/Mole). For this field, the
 five nitrogen species must be in the order N, N₂, N⁺, e⁻, N₂⁺.

Line 3, 5, 7, ..., 2*JE+1, (One for each spatial location starting with the point
 closest to the body) [6E13.6]

Field 1, (Columns 1-13) ETA(j)
 Nondimensional spatial location at the jth spatial point,
 $ETA(j) = Y/Y_{shock}$.

Field 2, (Columns 14-26) RHO(j,2)
 Nondimensional density at the jth spatial point,
 $RHO(j,2) = \rho/(RHOREF*RS(2))$.

Field 3, (Columns 27-39) P(j,2)
 Nondimensional pressure at the jth spatial point,
 $P(j,2) = P/(PREF*PS(2))$.

Field 4, (Columns 40-52) T(j,2)
 Nondimensional temperature at the jth spatial point,
 $T(j,2) = T/TREF$.

Field 5, (Columns 53-65) TE(j)
 Nondimensional electron/electronic temperature at the jth spatial
 point, $TE(j) = T_e/TREF$.

Field 6, (Columns 66-78) EMBAR(j)
 Molecular weight of the gas at the jth spatial point, (g/Mole).

Line 4, 6, 8, ..., 2*JE+2, (One for each spatial location starting with the point
 closest to the body) [12E13.6]

Field 1, 2, ..., NS, (Columns 1-13, 14-26, etc) (CC(j,2,k), k=1, NS)
 Mass fraction for the kth species at the jth spatial location,
 $CC(j,2,k) = \rho_k/\rho$. The five nitrogen species must be in the same
 order as the molecular weights in line 2.

prec.dat - Precursor flow field data, see Appendix C.

Line 1, [I5] JPREC
 The number of spatial points used in the precursor, maximum of
 $JE + JPREC = 300$.

Line 2, 4, 6, ..., 2*JPREC, (One for each spatial location starting with the point closest to the body) [6E13.6]

Field 1, (Columns 1-13) ETA(j)

Nondimensional spatial location at the jth spatial point,
 $\text{ETA}(j) = Y/Y_{\text{shock}}$.

Field 2, (Columns 14-26) RHO(j,2)

Nondimensional density at the jth spatial point,
 $\text{RHO}(j,2) = \rho / (\text{RHOREF} * \text{RS}(2))$.

Field 3, (Columns 27-39) P(j,2)

Nondimensional pressure at the jth spatial point,
 $\text{P}(j,2) = P / (\text{PREF} * \text{PS}(2))$.

Field 4, (Columns 40-52) T(j,2)

Nondimensional temperature at the jth spatial point,
 $\text{T}(j,2) = T / \text{TREF}$.

Field 5, (Columns 53-65) TE(j)

Nondimensional electron/electronic temperature at the jth spatial point, $\text{TE}(j) = T_e / \text{TREF}$.

Field 6, (Columns 66-78) EMBAR(j)

Molecular weight of the gas at the jth spatial point, (g/Mole).

Line 3, 5, 7, ..., 2*JPREC+1, (One for each spatial location starting with the point closest to the body) [12E13.6]

Field 1, 2, ..., NS, (Columns 1-13, 14-26, etc) (CC(j,2,k), k=1, NS)

Mass fraction for the kth species at the jth spatial location,
 $\text{CC}(j,2,k) = \rho_k / \rho$. The five nitrogen species must be in the same order as the molecular weights in line 2.

rad.dat - Permanent and case specific data for the radiation calculations. Details of this input file are presented in reference 3 and an example of this file is shown in Appendix D. Changes to the description in reference 3 are as follows.

DECK B - CASE DATA

Group 1 - Control Card and Title

Card 1, [20I1, 15A4]

Field 1, (Columns 1-20) KR

Column 14 - Determines whether local thermodynamic nonequilibrium corrections are used in the shock layer.

- 0 - No LTNE corrections
- 1 - Using LTNE corrections

Column 15 - Determines whether local thermodynamic nonequilibrium corrections are used in the precursor.

- 0 - No LTNE corrections
- 1 - Using LTNE corrections

fort.3 - Species excited state data and transition cross sections used in calculating collision limiting LTNE correction factors in the precursor region.

OUTPUT FILES

radical.out - Detailed output from the radiative transfer calculations. A discussion of this output is given in reference 3.

fort.55 - Precursor flow field properties for input into the program PREC. NOTE: This is an unformatted file and can not be printed or viewed on the screen.

fort.56 - Spectrally detailed data from the radiative transfer calculations for input into the program PREC. NOTE: This is an unformatted file and can not be printed or viewed on the screen.

PREC

The program, PREC, utilizes the results of the radiative transfer calculations by RADICAL and calculates the flow field conditions in the precursor. This program treats the precursor as a nitrogen gas and includes the effects of chemical as well as thermal nonequilibrium. Thermal nonequilibrium is accounted for in this program through the inclusion of an electron/electronic temperature and appropriately an electron/electronic energy equation. A variable spatial step size is also utilized to force the property changes between each spatial point to remain within user provided limits. A detailed discussion of this precursor model and the solution scheme used in this program is provided in reference 1.

INPUT FILES

prec.inp - Thermodynamic data for the precursor calculations. An example of this input file is provided in Appendix E.

Line 1, [A5] Dummy line, not used.

Line 2, [E12.4] DH
Planck's constant, (erg-sec).

Line 3, [E12.4] R
Universal gas constant, (erg/(Mole °K)).

Line 4, [E12.4] AV
Avogadro's number, (1/Mole).

Line 5, [E12.4] C
Speed of light, (cm/sec).

Line 6, [A5] Dummy line, not used.

Line 7, [E12.4] VIN
Freestream velocity, (cm/sec).

Line 8, [E12.4] RBODY
Body radius, (cm).

Line 9, [E12.4] YSHOCK
Shock standoff distance, (cm).

Line 10, [I2] NCORR

Radiation correction flag, specifies which method, if any, should be used to account for the geometric attenuation of the radiation in the precursor, see Appendix C of reference 1.

- 0 - No geometric attenuation
- 1 - Include geometric attenuation using body attenuation factor
- 2 - Include geometric attenuation using shock layer attenuation factor

Line 11, [I2] NDBG

Debug flag, specifies whether extended files are created to aid in debugging problems in the code.

- 0 - No extended output
- 1 - Create extended output

Using the "1" option for this flag creates six files in addition to the standard output files.

fort.15 - Contains the mass production rate for each species at each spatial location. The first column contains the spatial location and the following five columns are the production rates for the five species: N, N₂, N⁺, e⁻, N₂⁺.

fort.16 - Contains the values for the terms on the right hand side of the electron/electronic energy equation. These terms are in the order of the terms in equation (7) of reference 1 where the last two terms have been combined.

fort.18 - Contains detailed output of the temperature and the mass fractions during the iteration at each spatial location.

fort.19 - Contains details about the integral terms on the right hand side of the electron/electronic energy equation and the portions of these terms due to each individual molecular band.

fort.75 - Contains the spatial and frequency variation of the geometric attenuation factors.

fort.76 - Contains the spatial and frequency variations of the total absorption coefficient.

Line 12, [A5] Dummy line, not used.

Line 13, [A5] Dummy line, not used.

Line 14, [I2] NS

Number of species.

Line 15, 21, ..., 9+NS*6, [A5] SPECSYM(i)

Periodic symbol for the ith species.

Line 16, 22, ..., 10+NS*6, [3E10.4]

Field 1, (Columns 1-10) MW(i)

Molecular weight for the ith species, (g/Mole).

Field 2, (Columns 11-20) EION(i)

Ionization energy for the ith species, (ev).

Field 3, (Columns 21-30) EDISS(i)

Dissociation energy of the ith species, (ev).

Line 17, 23, ..., 11+NS*6, [3F8.4]

Field 1, (Columns 1-8) TRAROT(i)

Constant for the translational/rotational energy relation. Ie.

3/2 for N

5/2 for N₂

Field 2, (Columns 9-16) THTVIBR(i)

Characteristic temperature of vibration for the ith species, (°K).

Field 3, (Columns 17-24) EZERO(i)

Zero point energy of the ith species, (ev).

Line 18, 24, ..., 12+NS*6, [I2] NEL(i)

Number of electronic levels included in the electronic energy term for the ith species.

Line 19, 25, ..., 13+NS*6, [10F10.4]

Field 1, 2, ..., NEL(i), (Columns 1-10, 11-20, etc)

(DEG(i,j), j=1, NEL(i))

Degeneracy for the jth electronic state of the ith species.

Line 20, 26, ..., 14+NS*6 [10F10.4]

Field 1, 2, ..., NEL(i), (Columns 1-10, 11,20, etc)

(THTEL(i,j), j=1, NEL(i))

Characteristic temperature for the jth electronic state of the ith species, (°K).

Line 15+NS*6, [A5] Dummy line, not used.

Line 16+NS*6, [A5] Dummy line, not used.

Line 17+NS*6, [I3] NCOL

Number of sets of collision cross section data included below.

Line 18+NS*6, 19+NS*6, ..., 17+NS*6+NCOL, [2I2, 2F10.4]

Field 1, (Columns 1-2) NS1

Number for the first species involved in the reaction associated with the following collision cross section data. NOTE: NS1 < NS2.

Field 2, (Columns 3-4) NS2

Number for the second species involved in the reaction associated with the following collision cross section data.

NOTE: NS1 < NS2.

Field 3, (Columns 5-14) VLG2000

Value of the logarithm₁₀ of the collision cross section at 2000°K.

NOTE: This program assumes the collision cross sections are given as a linear variation of the logarithm₁₀ of the cross section as given in Gnoffo, Gupta and Shinn⁵.

Field 4, (Columns 15-24) VLG4000

Value of the logarithm₁₀ of the collision cross section at 4000°K.

prec.conv - Convergence criteria for the precursor calculations. An example of this file is shown in Appendix E.

Line 1, [3(F6.4, 1X), I1, 1X, F6.4]

Field 1, (Columns 1-6) VLCONV

Convergence criteria for the local iteration at each point in the precursor expressed as a maximum fractional change. Ie.

$$\frac{(V^{n+1} - V^n)}{V^n} \leq VLCONV$$

Field 2, (Columns 8-13) DELMX

Maximum fractional change between each spatial point for the variable spacing.

Field 3, (Columns 15-20) DELMN

Minimum fractional change between each spatial point for the variable spacing.

Field 4, (Column 22) NELCT
Flag controlling thermal nonequilibrium.

0 - Thermal equilibrium
1 - Thermal nonequilibrium

Field 5, (Columns 24-29) DAMP
Not used in this program.

fort.55 - Precursor flow field properties from previous iteration. This file is created by the program RADICAL. NOTE: This is an unformatted file and can not be printed or viewed on the screen.

fort.56 - Spectrally detailed data from the radiative transfer calculations created by the program RADICAL. NOTE: This is an unformatted file and can not be printed or viewed on the screen.

OUTPUT FILES

fort.11 - Precursor flow field conditions in a form suitable for input into a graphing program.

Line 1, 2, ..., [14(E16.9, 1X)]
Field 1, (Columns 1-16) ETAS(k)
Nondimensional spatial distance from the body, Y/Y_{shock} .

Field 2, (Columns 18-33) QTOTS(K)
Radiative flux corrected for the geometric attenuation, (W/cm^2).

Field 3, (Columns 35-50) VELOS(k)
Velocity, (cm/sec).

Field 4, (Columns 52-67) TEMPS(k)
Heavy particle temperature, ($^{\circ}\text{K}$).

Field 5, (Columns 69-84) PRESS(k)
Pressure, (dyn/cm^2).

Field 6, (Columns 86-101) DENSS(k)
Density, (g/cm^3).

Field 7, (Columns 103-118) EE
Electron/electronic energy, (erg/g).

Field 8, (Columns 120-135) PHTS(k)
Total enthalpy, (erg/g).

Field 9, (Columns 137-152) MASFS(1,k)
N mass fraction.

Field 10, (Columns 154-169) MASFS(2,k)
N₂ mass fraction.

Field 11, (Columns 171-186) MASFS(3,k)
N⁺ mass fraction.

Field 12, (Columns 188-203) MASFS(4,k)
e⁻ mass fraction.

Field 13, (Columns 205-220) MASFS(5,k)
N₂⁺ mass fraction.

Field 14, (Columns 222-237) TES(k)
Electron/electronic temperature, (°K).

prec.dat - Precursor flow field data in the format suitable for input into the program RADICAL. The format of this file follows that given for the input file by this name under the program RADICAL.

CHKCONV

This program reads two sets of precursor flow field data and calculates the maximum change in each flow field variable and creates an output file with this iteration data. If the maximum fractional change is less than an input global convergence criteria then a file, "converged", is created indicating that a converged precursor solution has been obtained.

INPUT FILES

prec.conv - This file contains the global iteration number and convergence criteria.
An example of this file is given in Appendix F.

Line 1, [3(F6.4, 1X), I1, 1X, 2(F6.4, 1X), I2]

Field 1, (Columns 1-6) VLCONV

Not used in this program.

Field 2, (Columns 8-13) DELMX

Not used in this program.

Field 3, (Columns 15-20) DELMN

Not used in this program.

Field 4, (Column 22) NELCT

Not used in this program.

Field 5, (Columns 24-29) DAMP

Damping coefficient for the changes in the electron/electronic temperature between each iteration. Ie.

$$T_e^{n+1} = T_e^n + (T_e^{n+1} - T_e^n) DAMP$$

Field 6, (Columns 31-36) GCONV

Global convergence criteria in maximum fractional change allowed for convergence. This is applied to all flow field variables.

Field 7, (Columns 38-39) NIT

Global iteration number. Each time CHKCONV is executed this number is incremented by one.

prec.dat - Current precursor flow field properties. This file is in the same format as the input file by the same name under the program RADICAL.

prec.dat.old - Precursor flow field properties from the previous global iteration. This file is in the same format as the file "prec.dat" above. It should be noted that this file should be copied from the "prec.dat" file immediately prior to running PREC since this program creates a new "prec.dat" file, see Appendix A.

OUTPUT FILES

prec.conv - This file contains the global convergence criteria and the global iteration number; it is identical to the input file by the same name except the iteration number is incremented by one.

prec.dat - This file contains the output precursor flow field conditions and is identical to the input file, "prec.dat", except that the damping coefficient has been applied to the change in the electron/electronic temperature as discussed under the input file, "prec.conv".

preciter.out - This file contains the iteration information regarding the maximum change in each of the flow field properties through each global iteration. An example of this file is shown in Appendix G.

converged - This file is created when a converged precursor solution is obtained. It contains the iteration number on which convergence was obtained and each successive iteration number following convergence.

MISCELLANEOUS TOOLS

The four programs described in this section are tools which were developed to help work with the precursor codes. One of these programs creates an input "prec.dat" file for beginning a precursor solution and the remaining three programs extract useful data from the unformatted files, "fort.55" and "fort.56".

MKPRECIN - This program prompts the user for the freestream conditions, the number of spatial points desired in the precursor, the desired spatial extent of the precursor data file in terms of Y/Y_{shock} as well as the reference and shock conditions from the first line of the "fort.24" file. It then creates an output file, "prec.dat.save", which has the proper freestream conditions and is in the format for use as an initial "prec.dat" file to begin a precursor solution. This file, however, should be edited by hand and more points should be added near the shock. Appendix C shows an initial "prec.dat" file with a suitable distribution of spatial points near the shock.

Input Data

JPREC - Number of spatial points in the precursor.

ETAMAX - Maximum Y/Y_{shock} value desired in "prec.dat" file.

Freestream Conditions

T - Freestream temperature, ($^{\circ}\text{K}$).

ρ - Freestream density, (g/cm^3).

Reference Conditions

Same as given in discussion of "fort.24" input file under the program RADICAL.

RFREQ - This program reads the "fort.55" and "fort.56" files and creates a file, "freq.dat", containing the spectral variation of the radiative flux at up to ten user selected spatial points in the precursor.

RFREQX - This program reads the "fort.55" and "fort.56" files and creates a file, "freq.dat", containing the spatial variation of the radiative flux in the precursor at up to fifteen frequencies selected by the user.

RDELQALL - This program reads the "fort.55" and "fort.56" files and creates an output file, "fort.81", which contains the change in the radiative flux, Δq_{ν} , between each spatial point for all frequencies. This is useful since the sign of this value indicates whether absorption or emission occurs. If the sign is positive, absorption occurs between the two spatial points at the particular frequency. If the sign is negative, emission occurs.

REFERENCES

1. Stanley, S.A., "The Effects of Shock Wave Precursors Ahead of Hypersonic Entry Vehicles", Masters Thesis, Texas A&M University, College Station, TX, Dec. 1990.
2. Nicolet, W.E., "Advanced Methods for Calculating Radiation Transport in Ablation-Product Contaminated Boundary Layers", NASA-CR-1656, Sept. 1970.
3. Nicolet, W.E., "User's Manual for the Generalized Radiation Transfer Code (RAD/EQUIL)", NASA-CR-116353, Oct. 1969.
4. Horton, T.E., "Radiative Coupled Nonequilibrium Flow Fields Associated with Aeroassisted Orbital Transfer", Final Contractors Report, NASA Grant NAG-1-496, March 1986.
5. Gnoffo, P.A., Gupta, R.N. and Shinn, J.L., "Conservation Equations and Physical Models for Hypersonic Air Flows in Thermal and Chemical Nonequilibrium", NASA-TN-2867, Feb. 1989.

APPENDIX A: command file

```
# radical
mv radical.out rad.out
mv prec.dat prec.dat.old
prec
mv fort.11 prec1.dat
chkconv

radical
mv radical.out rad.out
mv prec.dat prec.dat.old
prec
mv fort.11 prec2.dat
chkconv

radical
mv radical.out rad.out
mv prec.dat prec.dat.old
prec
mv fort.11 prec3.dat
chkconv

radical
mv radical.out rad.out
mv prec.dat prec.dat.old
prec
mv fort.11 prec4.dat
chkconv

radical
mv radical.out rad.out
mv prec.dat prec.dat.old
prec
mv fort.11 prec5.dat
chkconv
```

APPENDIX B: fort.24

51	0.000000E+00	0.315174E-01	0.754600E+01	0.443041E+06	0.742185E+00	0.874496E+00	0.387860E-07
0.795348E+01	0.670367E-02						
5	0.140200E+02	0.280400E+02	0.140200E+02	0.548600E-03	0.280400E+02		
0.000000E+00	0.308872E+02	0.112838E+01	0.670367E-02	0.670367E-02	0.138912E+02		
0.986031E+00	0.312954E-02	0.108388E-01	0.424125E-06	0.179520E-06			
0.508404E-02	0.128738E+02	0.112834E+01	0.160825E-01	0.160881E-01	0.138907E+02		
0.986011E+00	0.312113E-02	0.108669E-01	0.425222E-06	0.179593E-06			
0.106765E-01	0.102332E+02	0.112834E+01	0.202268E-01	0.202345E-01	0.137622E+02		
0.977474E+00	0.252945E-02	0.199951E-01	0.782415E-06	0.599138E-06			
0.168282E-01	0.873712E+01	0.112834E+01	0.236824E-01	0.236917E-01	0.136094E+02		
0.967082E+00	0.182671E-02	0.310885E-01	0.121651E-05	0.115785E-05			
0.235950E-01	0.774400E+01	0.112834E+01	0.267116E-01	0.267222E-01	0.134402E+02		
0.955060E+00	0.119887E-02	0.437376E-01	0.171148E-05	0.178235E-05			
0.310385E-01	0.702004E+01	0.112834E+01	0.294599E-01	0.294714E-01	0.132568E+02		
0.941323E+00	0.734029E-03	0.579386E-01	0.226718E-05	0.255744E-05			
0.392264E-01	0.646648E+01	0.112834E+01	0.319774E-01	0.319897E-01	0.130601E+02		
0.925828E+00	0.443805E-03	0.737217E-01	0.288479E-05	0.363211E-05			
0.482331E-01	0.603256E+01	0.112834E+01	0.342751E-01	0.342878E-01	0.128508E+02		
0.908575E+00	0.288181E-03	0.911278E-01	0.356591E-05	0.505785E-05			
0.581405E-01	0.568937E+01	0.112834E+01	0.363414E-01	0.363540E-01	0.126294E+02		
0.889559E+00	0.211592E-03	0.110219E+00	0.431297E-05	0.668531E-05			
0.690386E-01	0.541875E+01	0.112833E+01	0.381557E-01	0.381676E-01	0.123963E+02		
0.868741E+00	0.170233E-03	0.131075E+00	0.512912E-05	0.821278E-05			
0.810264E-01	0.520757E+01	0.112833E+01	0.397025E-01	0.397131E-01	0.121523E+02		
0.846074E+00	0.140574E-03	0.153770E+00	0.601716E-05	0.933933E-05			
0.942131E-01	0.504470E+01	0.112832E+01	0.409838E-01	0.409925E-01	0.118991E+02		
0.821561E+00	0.114451E-03	0.178307E+00	0.697732E-05	0.990368E-05			
0.108718E+00	0.491960E+01	0.112831E+01	0.420255E-01	0.420319E-01	0.116396E+02		
0.795332E+00	0.909578E-04	0.204559E+00	0.800456E-05	0.992604E-05			
0.124674E+00	0.482227E+01	0.112830E+01	0.428731E-01	0.428773E-01	0.113784E+02		
0.767707E+00	0.709796E-04	0.232203E+00	0.908625E-05	0.955369E-05			
0.142226E+00	0.474404E+01	0.112828E+01	0.435791E-01	0.435816E-01	0.111212E+02		
0.739232E+00	0.550023E-04	0.260694E+00	0.102011E-04	0.896848E-05			
0.161532E+00	0.467850E+01	0.112825E+01	0.441883E-01	0.441898E-01	0.108745E+02		
0.710648E+00	0.427982E-04	0.289289E+00	0.113200E-04	0.831694E-05			
0.182770E+00	0.462180E+01	0.112821E+01	0.447287E-01	0.447297E-01	0.106445E+02		
0.682802E+00	0.337352E-04	0.317144E+00	0.124099E-04	0.768767E-05			
0.206131E+00	0.457200E+01	0.112814E+01	0.452133E-01	0.452142E-01	0.104359E+02		
0.656484E+00	0.270935E-04	0.343469E+00	0.134400E-04	0.712183E-05			
0.231828E+00	0.452811E+01	0.112806E+01	0.456481E-01	0.456487E-01	0.102507E+02		
0.632222E+00	0.222257E-04	0.367735E+00	0.143895E-04	0.663057E-05			
0.260095E+00	0.448925E+01	0.112794E+01	0.460382E-01	0.460386E-01	0.100877E+02		
0.610122E+00	0.186042E-04	0.389838E+00	0.152544E-04	0.620773E-05			
0.291188E+00	0.445428E+01	0.112777E+01	0.463926E-01	0.463927E-01	0.994259E+01		
0.589844E+00	0.158238E-04	0.410119E+00	0.160480E-04	0.583825E-05			
0.325391E+00	0.442192E+01	0.112753E+01	0.467225E-01	0.467223E-01	0.981001E+01		
0.570788E+00	0.135963E-04	0.429177E+00	0.167937E-04	0.550469E-05			
0.363014E+00	0.439105E+01	0.112721E+01	0.470373E-01	0.470370E-01	0.968527E+01		
0.552383E+00	0.117392E-04	0.447582E+00	0.175139E-04	0.519292E-05			
0.404400E+00	0.436094E+01	0.112676E+01	0.473431E-01	0.473424E-01	0.956560E+01		
0.534274E+00	0.101506E-04	0.465692E+00	0.182226E-04	0.489466E-05			
0.449924E+00	0.433115E+01	0.112613E+01	0.476424E-01	0.476412E-01	0.944971E+01		
0.516301E+00	0.877486E-05	0.483667E+00	0.189259E-04	0.460620E-05			
0.500000E+00	0.430126E+01	0.112527E+01	0.479366E-01	0.479345E-01	0.933696E+01		
0.498385E+00	0.757591E-05	0.501583E+00	0.196269E-04	0.432581E-05			
0.550076E+00	0.427297E+01	0.112408E+01	0.482032E-01	0.482002E-01	0.923634E+01		
0.482028E+00	0.661362E-05	0.517941E+00	0.202670E-04	0.407690E-05			
0.595600E+00	0.424696E+01	0.112263E+01	0.484361E-01	0.484323E-01	0.915364E+01		
0.468314E+00	0.590003E-05	0.531656E+00	0.208037E-04	0.387961E-05			
0.636986E+00	0.421892E+01	0.112106E+01	0.486897E-01	0.486851E-01	0.908563E+01		
0.456850E+00	0.539020E-05	0.543120E+00	0.212523E-04	0.374978E-05			
0.674609E+00	0.417596E+01	0.111924E+01	0.491113E-01	0.491049E-01	0.903283E+01		
0.447829E+00	0.513841E-05	0.552140E+00	0.216052E-04	0.376410E-05			
0.708812E+00	0.404871E+01	0.111684E+01	0.505463E-01	0.505380E-01	0.900251E+01		
0.442599E+00	0.563674E-05	0.557369E+00	0.218098E-04	0.443921E-05			
0.739905E+00	0.377744E+01	0.111338E+01	0.540201E-01	0.537974E-01	0.903469E+01		
0.448142E+00	0.825558E-05	0.551822E+00	0.215928E-04	0.709390E-05			
0.768172E+00	0.340284E+01	0.110820E+01	0.597263E-01	0.587972E-01	0.916790E+01		
0.470669E+00	0.169101E-04	0.529278E+00	0.207108E-04	0.149054E-04			
0.793869E+00	0.291357E+01	0.109969E+01	0.693585E-01	0.658027E-01	0.943155E+01		
0.513341E+00	0.521685E-04	0.486545E+00	0.190393E-04	0.427395E-04			
0.817230E+00	0.228998E+01	0.108582E+01	0.876423E-01	0.741249E-01	0.988340E+01		

0.580927E+00 0.214925E-03 0.418665E+00 0.163857E-04 0.177483E-03
0.838468E+00 0.174610E+01 0.106781E+01 0.114029E+00 0.794938E-01 0.104968E+02
0.662478E+00 0.772377E-03 0.336040E+00 0.131628E-04 0.696067E-03
0.857774E+00 0.143235E+01 0.104974E+01 0.137656E+00 0.807715E-01 0.110897E+02
0.730893E+00 0.206527E-02 0.265278E+00 0.104146E-04 0.175365E-02
0.875326E+00 0.124915E+01 0.103409E+01 0.156469E+00 0.800122E-01 0.116025E+02
0.781261E+00 0.468934E-02 0.210716E+00 0.831034E-05 0.332608E-02
0.891282E+00 0.113103E+01 0.102084E+01 0.171744E+00 0.782420E-01 0.120490E+02
0.816190E+00 0.985404E-02 0.168518E+00 0.670035E-05 0.543067E-02
0.905787E+00 0.104655E+01 0.100932E+01 0.185134E+00 0.756468E-01 0.124616E+02
0.837388E+00 0.196406E-01 0.134884E+00 0.543610E-05 0.808225E-02
0.918974E+00 0.980817E+00 0.998897E+00 0.198014E+00 0.720397E-01 0.128776E+02
0.844562E+00 0.370918E-01 0.107264E+00 0.441396E-05 0.110782E-01
0.930961E+00 0.926934E+00 0.989341E+00 0.211488E+00 0.667324E-01 0.133395E+02
0.835932E+00 0.661117E-01 0.840770E-01 0.356139E-05 0.138757E-01
0.941860E+00 0.883674E+00 0.980966E+00 0.226130E+00 0.588362E-01 0.138983E+02
0.808716E+00 0.111182E+00 0.643466E-01 0.282607E-05 0.157529E-01
0.951767E+00 0.853005E+00 0.974458E+00 0.241937E+00 0.489825E-01 0.146163E+02
0.759615E+00 0.176645E+00 0.475260E-01 0.217687E-05 0.162119E-01
0.960774E+00 0.835590E+00 0.970355E+00 0.259010E+00 0.396633E-01 0.155528E+02
0.686922E+00 0.264236E+00 0.335643E-01 0.161224E-05 0.152760E-01
0.968961E+00 0.830089E+00 0.968787E+00 0.277616E+00 0.321215E-01 0.167398E+02
0.593813E+00 0.370213E+00 0.226315E-01 0.114659E-05 0.133415E-01
0.976405E+00 0.835297E+00 0.969713E+00 0.297752E+00 0.262578E-01 0.181924E+02
0.486845E+00 0.487777E+00 0.145404E-01 0.780999E-06 0.108375E-01
0.983172E+00 0.851839E+00 0.973205E+00 0.319103E+00 0.217103E-01 0.199468E+02
0.371429E+00 0.611762E+00 0.875255E-02 0.500108E-06 0.805640E-02
0.989324E+00 0.882272E+00 0.979443E+00 0.341202E+00 0.181049E-01 0.220811E+02
0.250575E+00 0.739534E+00 0.469990E-02 0.285457E-06 0.519047E-02
0.994916E+00 0.930296E+00 0.988483E+00 0.363589E+00 0.153624E-01 0.247184E+02
0.126200E+00 0.869456E+00 0.191639E-02 0.122495E-06 0.242819E-02
0.100000E+01 0.100000E+01 0.100000E+01 0.385923E+00 0.153624E-01 0.280400E+02
0.000000E+00 0.100000E+01 0.000000E+00 0.000000E+00 0.000000E+00

APPENDIX C: prec.dat

APPENDIX D: rad.dat

2056

0.40	+01	0.10	+02	0.60	+01	0.18	+02	0.54	+02	0.90	+02
0.00	+00	0.00	+00	0.90	+01	0.50	+01	0.10	+01	0.50	+01
0.30	+01	1.50	+01	0.90	+01	0.40	+02	0.90	+01	0.50	+01
0.10	+01	0.50	+01	0.12	+02	0.15	+02	0.36	+02	0.00	+00
0.20	+01	0.80	+01	0.18	+02	0.32	+02	0.00	+00	0.00	+00
0.00	+00	0.00	+00	0.90	+01	0.00	+00	0.00	+00	0.00	+00
0.00	+00	0.00	+00	0.00	+00	0.00	+00	0.40	+01	0.00	+00
0.00	+00	0.00	+00	0.00	+00	0.00	+00	0.00	+00	0.00	+00
0.60	+01	0.00	+00	0.00	+00	0.00	+00	0.00	+00	0.00	+00
0.00	+00	0.00	+00	0.00	+00	0.00	+00	0.00	+00	0.00	+00
0.00	+00	0.2384+01		0.3576+01		0.1045+02		0.1188+02		0.1300+02	
0.00	+00	0.00	+00	0.96	-02	0.1967+01		0.4189+01		0.9144+01	
0.9519+01		0.1074+02		0.1099+02		0.1208+02		0.00	+00	1.2639+00	
2.6839+00		4.1825+00		7.5351+00		7.9461+00		8.6442+00		0.00	+00
0.00	+00	0.1020+02		0.1208+02		0.1274+02		0.00	+00	0.00	+00

0

0.60	+00	0.85	+00	0.96	+00	0.12	+01	0.14	+01	0.162	+01
0.24	+01	0.34	+01	0.62	+01	0.80	+01	0.86	+01	0.90	+01
0.97	+01	0.1045	+02	0.1080	+02	0.1170	+02	0.1210	+02	0.1280	+02
0.1340	+02	0.1380	+02	0.00	+00	0.00	+00	0.00	+00	0.00	+00
0.80	+00	0.95	+00	0.12	+01	0.14	+01	0.16	+01	0.24	+01
0.3340	+01	0.40	+01	0.80	+01	0.86	+01	0.90	+01	0.97	+01
0.1045	+02	0.1080	+02	0.1170	+02	0.1210	+02	0.1280	+02	0.1340	+02
0.1380	+02	0.1450	+02	0.00	+00	0.00	+00	0.00	+00	0.00	+00
0.69	+00	0.89	+00	0.1080	+01	0.1290	+01	0.1460	+01	0.1850	+01
0.2850	+01	0.3700	+01	0.7110	+01	0.8302	+01	0.8781	+01	0.94	+01
0.1007	+02	0.1062	+02	0.1120	+02	0.1190	+02	0.1241	+02	0.1304	+02
0.1358	+02	0.1420	+02	-	+	-	+	-	+	-	+

11	10.182	0.1510	653E-22		
1	10.332	0.1840	621E-22	12.	
3	10.418	0.0225	532E-20		
2	10.493	0.0187	446E-20		
3	10.585	0.0131	796E-20		
2	10.619	0.0533	312E-21	14.	
3	10.682	0.00819	268E-19		
3	10.757	0.00518	437E-19		
10	10.761	0.1200	653E-22		
1	10.927	0.4540	161E-23	12.	
11	11.007	0.0185	367E-21		
3	11.200	0.0200	446E-21		
2	11.293	0.0418	293E-20		
3	11.310	0.0254	323E-21		
33	11.424	0.2260	143E-23		
2	11.609	0.0250	532E-20		
2	11.776	0.0220	796E-20		
11	11.806	0.0049	145E-20		
09	11.852	0.0199	367E-21		
2	11.874	0.0091	268E-19		
2	11.948	0.00575	437E-19		
3	12.000	0.0269	299E-20		
09	12.067	0.0218	344E-21		
11	12.160	0.0019	128E-20		
3	12.316	0.0156	696E-20		
10	12.404	0.0461	653E-22		
2	12.414	0.0574	390E-21		
2	12.511	0.0279	337E-21		
09	12.521	0.0775	633E-22		
09	12.651	0.00524	145E-20		
1	12.877	0.0230	446E-21		
1	13.004	0.1320	294E-21	12.	
2	13.190	0.0489	299E-20		
2	13.508	0.0291	696E-19		
33	13.543	0.1610	950E-24		
1	13.677	0.0957	293E-20		
1	13.993	0.0584	532E-20		
1	14.160	0.0342	796E-20		
1	14.257	0.0212	268E-19		
1	14.332	0.0138	437E-19		
74					
.02	.1	.2	.3	.49	.6
.8	1.0	1.5	2.0	2.25	2.59
3.0	3.5	4.0	4.43	4.5	4.76
4.77	5.0	6.0	6.2	7.0	7.039
7.041	8.0	8.239	8.241	8.546	8.551
9.0	9.419	9.421	9.77	9.78	9.9
10.0	10.15	10.3	10.45	10.6	10.79
10.81	11.0	11.15	11.25	11.27	11.40
11.6	11.8	11.99	12.01	12.15	12.25
12.399	12.401	13.39	13.41	13.59	13.61
14.29	14.3	15.0	15.58	15.59	15.7
15.8	15.9	16.0	16.1	16.2	16.3
16.4	16.5				
10011010111201100000	FIRE II FLUX ABSORBED				
01100	1 0 1 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0				
1.					

APPENDIX E: prec.inp

APPENDIX F: prec.conv

0.0005 0.1500 0.0100 1 1.0000 0.0050 00

APPENDIX G: preciter.out

	dens	press	temp	eltemp	mf
nit= 1	damp= 1.0000	gconv= 0.0050			
del	- .1000000E-05	- .1217500E-04	- .9600000E-06	- .1728515E-01	0.2459000E-02
pdel	.7953361E-05	.5082998E-01	.1307991E-02	.2355085E+02	Inf
nit= 2	damp= 1.0000	gconv= 0.0050			
del	0.0000000E+00	0.8400000E-06	- .3130000E-06	0.2233700E-02	- .1300000E-04
pdel	.0000000E+00	.3362340E-02	.4259031E-03	.1410405E+00	Inf
nit= 3	damp= 1.0000	gconv= 0.0050			
del	0.1000000E-05	- .3200000E-07	0.1190000E-06	- .6180000E-04	- .1000000E-07
pdel	.7953298E-05	.1275475E-03	.1620165E-03	.4466189E-02	.2168221E-01
nit= 4	damp= 1.0000	gconv= 0.0050			
del	0.0000000E+00	0.2000000E-08	- .7000000E-08	0.1700000E-05	0.1000000E-07
pdel	.0000000E+00	.8274310E-05	.9531928E-05	.1225181E-03	.2498403E-03
nit= 5	damp= 1.0000	gconv= 0.0050			
del	0.0000000E+00	- .1000000E-08	0.2000000E-08	- .1000000E-06	0.2000000E-11
pdel	.0000000E+00	.4127422E-05	.2721829E-05	.7375556E-05	.7258738E-05